6.3. Efficiency Terms

6.3.01. Peak resolution ($R_{1/2}$) The definition of this term is identical to that given in 3.10.01.

$$R_{1/2} = \frac{V_{R1} - V_{R2}}{(w_{b1} + w_{b2})/2}$$

Here V_{R1} and V_{R2} represent the peaks corresponding to compounds with molecular masses M_1 and M_2 respectively: by definition $M_2 > M_1$. In exclusion chromatography, larger molecules are eluted first, therefore, $V_{R1} > V_{R2}$.

Because of the addition of a new term, the specific resolution (see 6.3.02), the symbol $R_{1/2}$ is suggested for peak resolution in exclusion chromatography.

6.3.02. Specific resolution (R_{sp}) Peak resolution also considering the molecular masses of the two test compounds:

$$R_{sp} = \frac{V_{R1} - V_{R2}}{(w_{b1} + w_{b2})/2} \frac{1}{\log(M_2/M_1)}$$

The test compounds used for the determination of the specific resolution should have a narrow molecular-mass distribution (the ratio of the mass-average and number-average molecular masses should be equal to or less than about 1.1) and differ by a factor of about 10 in their molecular masses.

Note: In some nomenclatures, the symbol R_s is used for the specific resolution. Due to the possibility of confusing it with the general resolution term (see 3.10.01), the symbol R_{sp} is suggested here.

6.3.03. Plate number and plate height (N, H) The definitions of these terms are identical to those given in 3.10.03 and 3.10.05.

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6.3.04. Effective plate number and effective plate height (N_{eff}, H_{eff}) The definitions of these terms are identical to those given in 3.10.04 and 3.10.06, except that the retention volume of a non-retained compound (V_o; see 6.2.01) is used in the calculations:

$$N_{eff} = 16\left[\frac{V_R - V_o}{w_b}\right]^2 = 5.545\left[\frac{(V_R - V_o)}{w_h}\right]^2$$

$$N_{eff} = 16\left[\frac{t_R - t_o}{w_b}\right]^2 = 5.545\left[\frac{(t_R - t_o)}{w_h}\right]^2$$

$$H_{eff} = L/N_{eff}$$

6.3.05. Reduced plate height (h) The definition of this term is identical to that given in 3.10.07.

12B. Liquid-Liquid Distribution (Solvent Extraction) (IUPAC Recommendations 1993)

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Abstract

The widespread use of liquid-liquid distribution, ranging from an analytical chemical technique to a unit operation in various fields of chemical technology (e.g. petroleum refining, nuclear fuel reprocessing, hydrometallurgy, food technology, biochemistry) has led to a proliferation of terminology. This paper extends the scope of the definitions beyond those previously recommended (*Pure Appl. Chem.* 1970, **21**, 111–113) and a list of terms, including those previously published, is presented under the following general headings: general definitions of phenomena, operations and relationships; components of the solvent phase; fundamental parameters for quantitative description of liquid-liquid distribution systems; process terminology applicable to large scale continuous operations.

Introduction

In 1970 IUPAC published 'Recommended Nomenclature for Liquid-Liquid Distribution' [1] which represented the work of several generations of the Nomenclature Commission V.3 of the International Union of Pure and Applied Chemistry, assisted by the work of an *ad hoc* working party which considered the whole of the nomenclature of separation processes. The choice of terms selected for definition was somewhat arbitrarily restricted to those commonly used in what might be termed small scale batch or laboratory analytical procedures. Many requests were received to extend the range of terms defined and the need for a complete revision was emphasized by the publication independently of other nomenclature proposals [2–5].

The wide variation [6] in the choice of symbols and in nomenclature adopted by authors of papers published in the Proceedings of the International Conferences on Solvent Extraction in Gothenburg (1966) and in Scheveningen (1971) convinced the organizing committee of the next conference at Lyons (ISEC-1974) of the desirability of providing authors with an extensive set of recommendations in order to aim at consistency in nomenclature and symbols in the published proceedings. These were drawn up by a working party of the Solvent Extraction and Ion Exchange Group of the Society of Chemical Industry (SCI), after meetings at Bradford and Birmingham (England) attended by representatives of all aspects of the field. Their report, drawn up by Dr Rice (as Secretary) formed the basis of discussions at the IUPAC General Assembly held in Munich during August 1973. This led to a new set of recommendations which were made available for comment at ISEC-74. After further discussions at a meeting of Commission V.3 of IUPAC in London in November 1974 and at the IUPAC General Assembly in Madrid in 1975, a tentative document was issued as an Information Bulletin [7] by IUPAC in July 1977 and further discussed at the IUPAC General Assembly in Warsaw in August 1977. At almost the same time the Solvent Extraction and Ion Exchange Group of the SCI authorized publication of their considered proposals for Recommended Nomenclature for Solvent Extraction in *Chemistry in Industry* to coincide with the International Solvent Extraction Conference (ISEC-77) in Toronto [8]. A synthesis of all these proposals including the comments received on the tentative IUPAC proposals was discussed at the IUPAC General Assembly in Davos in September 1979, and circulated in draft form at ISEC-80 in Liege in September 1980, where some minor amendments to process terminology were proposed. Further discussion took place at Commission meetings in London in December 1980 and Leuven in September 1981.

These revised recommendations have been drawn up in collaboration with the Committee of the Solvent Extraction and Ion Exchange Group of the Society of Chemical Industry and have been discussed at several International Solvent Extraction Conferences.

Following the rearrangement of Commissions at the 35th IUPAC General Assembly in Lund in 1989, this project became the responsibility of the Limited Life Time Commission on Chromatography and Other Analytical Separations.

Since automated methods of analysis frequently simulate many of the features of large-scale industrial practice – not least in that the attainment of distribution equilibrium or quantitative extraction is not always achieved or even necessary – it seemed important in revising the original nomenclature to increase the scope of the terms previously defined so as to provide chemical engineers, clinical biochemists, food technologists, hydrometallurgists, nuclear technologists, petrochemists and physical as well as analytical chemists with a comprehensive set of symbols and nomenclature. In order to distinguish what might be termed 'processing' nomenclature, from that of a more fundamental nature, the recommendations have been placed in separate sections. However, the importance of achieving consistent usage and a common language for all users of

liquid-liquid extraction cannot be overstressed. The distinction between the two sets of terms is merely one of convenience and does not imply any real difference in their importance. In many instances, it is difficult to decide the appropriate category for a certain term so that the classification is somewhat arbitrary. Furthermore, some additional terms commonly used in the metallurgical industry have been added since publication of the tentative proposals [7].

In order to keep the definitions as general as possible the liquid phases involved have been designated as 'extract' or 'solvent' rather than 'organic phase' and 'other phase' or 'feed' rather than 'aqueous phase'. The need clearly to label and specify the relevant phase in any equations or graphs is emphasized. Symbols are recommended for a few of the more important parameters. The clear designation of the extract phase components is stressed; the term 'solvent' should be reserved for the composite phase rather than any individual component although it may be the only component in that phase. Terms which have become jargon in particular industrial situations or which may be confusing because of ambiguity have been listed as "not recommended". No attempt has been made to define standard chemical engineering terms, e.g. mass transfer coefficient, but certain terms, e.g. 'equilibrium constant' are discussed in relation to their usage in liquid-liquid distribution.

When the nomenclature is applied to other types of extraction systems (e.g. two immiscible aqueous phases, such as a concentrated salt solution and a concentrated aqueous solution of poly(ethylene glycol), two immiscible non-aqueous liquids or two immiscible molten salts), the two immiscible phases should be clearly specified and can equally well be distinguished and denoted by the general terms, Phase I and Phase II. It is also recognized that in the petrochemical and food-processing industries the extractant phase may well be an inorganic liquid (e.g. liquid sulfur dioxide, supercritical carbon dioxide). This situation can be described by using the terms "epi-phase" and "hypo-phase" for the less dense and more dense phases, respectively, recognizing that mass transfer could be in either direction. Occasionally, cases arise where metals are partitioned among three liquid phases, such as concentrated KCl, acetonitrile and hexane. The application of the recommended nomenclature to any situation is clearly a matter of common sense. What is important is that in a given situation the phases used should be completely specified.

Since the 'organic phase' is commonly quite a complex solution of one or more organic liquids containing one or more extractants and possibly 'modifiers' of various sorts as well as a 'diluent', particular care has been taken over the definitions applicable to these various components.

'Concentration' is frequently used in the list of definitions. In general any suitable concentration units may be employed but the *same* units should be used for each phase and should be clearly specified in the text.

Following normal convention, 'activities' rather than 'concentrations' should be used where thermodynamic equilibrium quantities are implied. However, use of the appropriate 'concentration quotient' as an approximation for the equilibrium constant in the limiting case of dilute solutions or in conjunction with the appropriate activity coefficients follows logically.

One semantic problem is the occurrence of three English terms – 'extraction', 'distribution' and 'partition' – to describe the transfer of a solute between phases whereas in many other languages only one suitable term exists (e.g. Verteilung). An attempt has been made to obviate this difficulty in the present work but its complete avoidance is not possible owing to established usage. The terms and symbols, which have been defined are listed in Tables 1 and 2, respectively. In some cases these represent changes, clarifications, or specific usages of previously defined terms [9], in particular those related to chromatographic separations [10], and the differences are not in Appendix 1.

The current reviser (MAL) suggests use of the term 'distribution' when referring to the total concentration of related species and 'partition' when referring to a single species. The term 'constant' should be reserved for fixed thermodynamic true constants, otherwise 'ratio' should be used. A survey of the literature shows reasonable agreement over the symbol and title of *partition constant* and *distribution ratio* but nomenclature for the *partition ratio* is a nightmare. Appendix 2 summarizes past usage.

1. General Definitions

1.1 Antagonism

The converse to *synergism* (1.23).

Note: The terms *anti-synergism*, *antisynergic* and *anti-synergistic* should not be used.

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1.2 Coextraction

Formation of mixed-species aggregates in a low-polarity organic phase.

1.3 Conditioning

A synonym for *pre-equilibration* (1.16).

1.4 Distribution

The apportionment of a solute between two phases.

Note: the term *partition* (1.15) or *extraction* (1.9) may also be used in this sense where appropriate.

1.5 Distribution Isotherm

The relationship (algebraic or graphical) between the concentration of a solute in the *extract* (2.7) and the corresponding concentration of the same solute in the other phase at equilibrium at a specified temperature.

Note: Alternative terms in common use are *equilibrium line* (1.7) and in the appropriate contexts: *extraction isotherm*, *scrubbing isotherm* and *stripping isotherm*. *Partition isotherm* is not normal usage.

1.6 Equilibration

The operation by which a system of two or more phases is brought to a condition where further changes with time do not occur.

Note: This term is not synonymous with *pre-equilibration* (1.16) and should not be used in that sense.

1.7 Equilibrium Line

A plot of the distribution isotherm (1.5).

1.8 Extract (Verb)

To transfer a solute from a liquid phase to another immiscible or partially miscible liquid phase in contact with it.

Notes:
(i) The term is also applied to the dissolution of material from a solid phase with a liquid in which it is not wholly soluble (i.e. *leaching*). See *solvent extraction* (1.19).
(ii) For usage as a noun see under '2 Components of the Solvent Phase'.

1.9 Extraction (in Liquid-liquid Distribution)

See *liquid-liquid extraction*.

Notes:
(i) See under '4 Process Terminology' for a more specific usage of *extraction*.
(ii) *Distribution* (1.4) and *partition* (1.15) are often used as synonyms for the general phenomenon of *extraction* where appropriate.

1.10 Liquid Ion Exchange

A term used to describe a liquid–liquid extraction process that involves a transfer of ionic species from the extractant to the aqueous phase in exchange for ions from the aqueous phase.

Notes:
(i) The term does not imply anything concerning the nature of the bonding in the extracted complex.
(ii) The term "*Solvent Ion Exchange*" (SIX) is not recommended.

1.11 Liquid-liquid Distribution (Extraction) (Partition)

The process of transferring a dissolved substance from one liquid phase to another (immiscible or partially miscible) liquid phase in contact with it.

Note: Although *extraction*, *partition* and *distribution* are not synonymous, *extraction* may replace *distribution* where appropriate.

1.12 Macro-element See *Main Solute*.

Notes:
(i) This term is vague and is not recommended.
(ii) Macroelement has a different meaning in analytical chemistry and the term *major component*, the meaning of which is obvious, is preferable.

1.13 Main (extractable) solute.

That (or those) species transferred which is of greatest economic or chemical interest.

Note: It is not necessarily the species present at greatest concentration.

1.14 Micro-element

This term should *not* be used in the sense of a minor component or a *contaminant* in the feed to a liquid-liquid distribution system.

Note: Microelement has a different meaning in analytical chemistry and the terms *minor component*, *impurity or contaminant* the meaning of which are obvious, are preferable.

1.15 Partition

This term is often used as a synonym for *distribution* (1.4) and *extraction* (1.9). However, an essential difference exists by definition between *distribution constant* or *partition ratio* (3.17) and *partition constant* (3.16).

Note: This term should be, but is not invariably, applied to the distribution of a single definite chemical species between the two phases.

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1.16 Pre-equilibration

(i) Preliminary treatment of a solvent in order to convert the extractants into a suitable chemical form.
(ii) Preliminary treatment of either phase with a suitable solution of the other phase (in the absence of *main extractable solute*(*s*) (1.13)) so that when the subsequent *equilibration* (1.6)) is carried out changes in the (volume) *phase ratio* (3.19) or in the concentrations of other components are minimised.

Notes:
(i) The use of *equilibration* (1.6) in this sense is confusing and should be avoided.
(ii) The term *conditioning* may be used as a synonym for *pre-equilibration*.

1.17 Re-extraction

Since the prefix 're-' can signify 'back' as well as 'again' this term is ambiguous and *should be avoided*, except where the process of extraction (e.g. from aqueous solution to an organic phase) in a single direction is repeated (following stripping). It should not be used as a synonym for *stripping* (4.3) or *back-extraction* (4.1).

1.18 Salting Out

The addition of particular electrolytes to an aqueous phase in order to increase the *distribution ratio* (3.5) of a particular solute.

Notes:
(i) The addition of electrolytes to improve phase separation behaviour should not be referred to as salting out.
(ii) The term is also used for the addition of electrolytes to reduce the mutual partial miscibility of two liquids.
(iii) It has no connection with *synergism* (1.23).

1.19 Solvent Extraction

The process of transferring a substance from any matrix to an appropriate liquid phase. If the substance is initially present as a solute in an immiscible liquid phase the process is synonymous with *liquid-liquid extraction* (1.11).

Notes:
(i) If the extractable material is present in a solid (such as a crushed mineral or an ore) the term *leaching* may be more appropriate. The extractable material may also be a liquid entrapped within or adsorbed on a solid phase.
(ii) Common usage has established this term as a synonym for *liquid–liquid distribution* (1.11). This is acceptable provided that no danger of confusion with extraction from solid phases exists in a given context.

1.20 Solvent Ion Exchange (SIX)

This term is not recommended (see *liquid ion exchange*) (1.10).

1.21 Sublation

A flotation process in which the material of interest, adsorbed on the surface of gas bubbles in a liquid, is collected on an upper layer of immiscible liquid.

Notes: There is no liquid-phase mixing in the bulk of the system; as a result recoveries can approach 100%.

1.22 Substoichiometric Extraction

Here the amount of reagent used is lower than that dictated by stoichiometry. If the constants of formation and extraction of the complexes are high, the amount of extracted metal is dictated by the amount of extractant introduced.

1.23 Synergism

A term describing the co-operative effect of two (or more) *extractants* (2.8) where the *distribution ratio* (3.5) for the combination is greater than the largest individual *distribution ratio* (measured under comparable conditions)

Notes:
(i) The corresponding adjective is *synergic* and the term *synergistic* should not be used.
(ii) No standard method for quantification of the phenomenon has been agreed and any approach should be clearly defined in a given situation.

2. Components of the Solvent Phase

2.1 Accelerator See *Catalyst (2.3), Kinetic Synergist (2.10), Modifier (2.11)*

Note: This term may be used as a synonym for catalyst.

2.2 Carrier See *Diluent (2.5)*

This term is not recommended.

2.3 Catalyst (in Liquid-liquid Distribution)

A substance included in the *solvent* (2.12) to increase the rate of transfer without affecting the position of equilibrium.

Notes: The term *accelerator* may also be used but *kinetic synergist* is not recommended.

2.4 Cosolvent See *Diluent (2.5)*

2.5 Diluent

The liquid or homogeneous mixture of liquids in which *extractant*(*s*) (2.8) and possible *modifier*(*s*) (2.11) may be dissolved to form the *solvent* (2.12) phase.

Notes:
(i) The term *carrier*, which implied an inert diluent is not recommended.
(ii) Although the diluent may well be a single liquid or even the major portion of the extracting phase, the term *solvent* (2.12) should not be used in this sense as it has a much wider meaning in the context of liquid-liquid extraction, although the term *cosolvent* may be used in certain circumstances.
(iii) The diluent by itself does not extract the *main* (*extractable*) *solute* appreciably

2.6 Epi-Phase

The less dense phase in a distribution system.

Note: The term is often used when two non-aqueous phases are present or when the *solvent* (2.12) is an aqueous solution. See also *hypo-phase* (2.9).

2.7 Extract (Noun)

The separated phase (often but not necessarily organic) that contains the material extracted from the other phase.

Notes:
(i) Where appropriate the term "*loaded solvent*" (4.15) may be used, but is not recommended.
(ii) For usage as a verb see 1.8.

2.8 Extractant

The active component(s) primarily responsible for transfer of a solute from one phase to the other.

Notes:
(i) The term *extracting agent* is a synonym but *solvent* (2.12) and *ligand* should not be used in this context.
(ii) Certain *extractants* that consist of liquids immiscible with water (e.g. Tributyl phosphate or certain ketones) might comprise the only component of the initial organic phase but *extractant*(*s*) can also be dissolved in *diluent* (2.5).

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2.9 Hypo-Phase

The denser phase in an extraction system.

Note: The term is often used when two non-aqueous phases are present or when the *solvent* (2.12) is an aqueous phase. See also *epi-phase* (2.6).

2.10 Kinetic Synergist

This term is not recommended as a synonym for *catalyst* (2.3) or *accelerator* (2.1).

2.11 Modifier

A substance added to a *solvent* (2.12) to improve its properties e.g. by increasing the solubility of an *extractant* (2.8), changing interfacial parameters, or reducing adsorption losses.

Note: Additives used to enhance extraction rates should be called *accelerators* (2.1) or *catalysts* (2.3).

2.12 Solvent (in Liquid-liquid Distribution)

The term applied to the whole initial liquid phase containing the *extractant* (2.8).

Notes:
(i) The solvent may contain only *extractant* or it may be a composite homogeneous mixture of *extractant*(*s*) (2.8) with *diluent*(*s*) (2.5) and also sometimes *modifiers* (2.11) and *accelerators* (2.1).
(ii) The term *solvent* must not be used as a synonym for any of the individual components of a composite liquid phase even where, in the case of a single component (e.g. 3-methylbutan-2-one or tributyl phosphate), it becomes identical with the *extractant*.
(iii) The term may be qualified to denote the *extract* from a given processing *step* (4.41), e.g. *loaded solvent* (4.15).

3. Fundamental Parameters

3.1 Concentration Factor

Not recommended. See *extraction factor* (3.10).

3.2 Decontamination Factor

The ratio of the proportion of contaminant to product before treatment to the proportion after treatment. It is the reciprocal of the *enrichment factor* (3.6).

3.3 Distribution Coefficient

This term is not recommended as a synonym for *distribution ratio* (3.5).

3.4 Distribution Constant

A synonym for *partition ratio* (3.17).

3.5 Distribution Ratio (in Liquid-liquid Distribution) (*D*)

The ratio of the total analytical concentration of a solute in the *extract* (2.7) (regardless of its chemical form) to its total analytical concentration in the other phase.

Notes:

(i) If there is possible confusion with the *extraction factor* or (*mass*) *distribution ratio* (3.13), the term *concentration distribution ratio* (symbol D_C) should be used, but this is not common usage. This is reasonably compatible with chromatographic nomenclature.

(ii) The terms *distribution coefficient*, *extraction coefficient* and, where appropriate, *scrubbing coefficient*, *stripping coefficient* are widely used alternatives but are not recommended. If they must be used in a given situation the term *ratio* is preferable to *coefficient*.

(iii) In equations relating to aqueous/organic systems the organic phase concentration is, by convention, the numerator and the aqueous phase concentration the denominator. In the case of *stripping ratio* the opposite convention is sometimes used but should then be clearly specified.

(iv) In the past there has been much confusion between the *distribution ratio* as defined above, the value of which varies with experimental conditions, e.g. pH, presence of complexing agents, extent of achievement of equilibrium, etc. and the true *partition constant* (3.16) which is by definition invariable or the *partition coefficient* or *distribution constant* which apply to a particular chemical species under specified conditions. For this reason the terms *distribution constant* (3.4), *partition constant* (3.16), *partition coefficient* (3.15), *partition ratio* (3.17) and *extraction constant* (3.9) should not be used in this context.

(v) The use of the ratio: *light phase concentration to heavy phase concentration* is ambiguous and is not recommended.

(vi) The *distribution ratio* is an experimental parameter and its value does not necessarily imply that distribution equilibrium between the phases has been achieved.

3.6 Enrichment Factor (in Liquid-liquid Distribution) (*S*)

The factor by which the ratio of the amounts of two substances in the *feed* (4.11) must be multiplied to give their ratio after treatment.

$Q_A/Q_B = S_{A,B}(Q'_A/Q'_B)$ where Q_A and Q'_A are the final and initial amounts of species A and Q_B and Q'_B are the final initial amounts of species B. Hence $S_{A,B} = E_A/E_B$ where E is the *fraction extracted* (3.11). In terms of D, n, r (where n is the number of stages and r the *phase ratio* (3.19))

$$S_{A,B} = \frac{1 - (1 + rD_A)^{-n}}{1 - (1 + rD_B)^{-n}}$$

3.7 Extractability

A property which qualitatively indicates the degree to which a substance is extracted.

Note: This term is imprecise and generally used in a qualitative sense. It is not a synonym for *fraction extracted* (3.11).

3.8 Extraction Coefficient

This term is not recommended as a synonym for *distribution ratio* (3.5).

3.9 Extraction (Equilibrium) Constant at Zero Ionic Strength (K^{o}_{ex})

The equilibrium constant of the distribution reaction expressed in terms of the reacting species. Thus, for the gross reaction:

$$M^{n+}_{aq} + n\,HL_{org} \rightleftharpoons ML_{n,org} + n\,H^{+}_{aq}$$

in which the reagent HL initially dissolved in an organic phase reacts with a metal ion M^{n+} in aqueous solution to form a product ML_n which is more soluble in the organic phase than in water,

$$K^{o}_{ex} = \frac{a_{MLn,org} \times a^{n}_{H^+,aq}}{a_{M^{n+},aq} \times a^{n}_{HL,org}}$$

Notes:

(i) When concentrations are used instead of activities or mixed terms are employed as when H^+ and/or M^{n+} are measured with an electrode, the appropriate name is *extraction constant*, symbol K_{ex}, accompanied by a careful definition. K^{o}_{ex} may be termed the *thermodynamic extraction constant*.

(ii) The extraction constant is related to other terms relevant to such systems by:

$$K_{ex} = \frac{D_{MLn}\,\beta_n\,K^{n}_{a}}{D^{n}_{HL}}$$

where β_n is the overall formation constant of ML_n and K_a is the dissociation constant of HL. When the reagent HL is more soluble in water than the other immiscible phase it may be more convenient to define a special equilibrium constant in terms of HL_{aq}:

$$K_{ex} = D_{ML,n}\,\beta_n\,K^{n}_{a}$$

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(iii) In distribution equilibria involving non-aqueous systems, e.g. liquid SO_2, molten salts and metals, the mass action equilibrium constant for the relevant extraction process can be identified with K_{ex} which should be explicitly defined in this context.

(iv) In actual practice, it may be necessary to include other terms to take into account other complexes formed by auxiliary reagents and the solvation and/or polymerization of the various species. In such cases, K_{ex} must be defined with reference to the relevant explicit chemical equation. An example is complex formation between the metal ion and an uncharged crown ether or cryptand molecule followed by ion-pair extraction:

$$M^{n+}_{aq} + L_{org} + nA^{-}_{aq} = (ML^{n+} \cdot A^{n-}_{n})_{org}$$

$$K_{ex} = \frac{[ML^{n+}A^{n-}_{n}]_{org}}{[M^{n+}]_{aq}[L]_{org}[A^{-}]^{n}_{aq}}$$

(v) Use of Ringbom's "conditional extraction constant",

$$K^{eff}_{ex} = \frac{a^{n}_{H^+} \cdot [ML'_n]_{org}}{[M']_{aq}[HL']^{n}_{org}}$$

in conjunction with alpha coefficients is useful [11].

(vi) The phases can also be specified by the formula of the solvent or by other symbols (preferably Roman numerals) or by overlining formulae referring to one phase, usually the less polar one. The subscript aq (or w) is often omitted; aq is preferable to w as the latter is appropriate only in English and German.

(vii) The qualification "Equilibrium" is often omitted.

(viii) The terms *partition constant and distribution constant* **must not** be used in this sense.

3.10 Extraction Factor (D_m)

The ratio of the total mass of a solute in the extract to that in the other phase.

Notes:
(i) It is the product of the (*concentration*) *distribution ratio* and the appropriate *phase ratio*.
(ii) It is synonymous with the *concentration factor* or *mass distribution ratio*, this latter term being particularly apt.
(iii) The term *concentration factor* is often employed for the overall *extraction factor* in a process or process step.

3.11 Fraction Extracted (E)

The fraction of the total quantity of a substance extracted (usually by the solvent) under specified conditions, i.e. $E_A = Q_A/Q'_A$ where Q_A is the mass of A extracted and Q'_A is the total mass of A present at the start.

Notes:
(i) E may be expressed as a percentage, $\%E$.
(ii) The term *extractability* is qualitative and should not be used as a synonym for *fraction extracted*.
(iii) If the aqueous phase is extracted with n successive portions of solvent, the phase volume ratio (solvent/feed) being r each time, the fraction extracted is given by:

$$E_n = 1 - (rD + 1)^{-n}$$

If $n = r = 1$, $E_1 = D/(1 + D)$ this expression is a concept of value in chromatography theory.
(iv) The fraction extracted is also known as the *recovery factor*, especially for a multistage process.

3.12 Loading Capacity

The maximum concentration of solute(s) that a *solvent* (2.12) can contain under specified conditions.

Notes:
(i) The terms *maximum loading*, *saturation capacity* and *saturation loading* are synonymous.
(ii) All the above terms should clearly be distinguished from *ultimate capacity* (3.29)

3.13 Mass Distribution Ratio See *Extraction Factor (3.10)*

3.14 Maximum Loading See *Loading Capacity (3.12)*

3.15 Partition Coefficient

This term is not recommended and should not be used as a synonym for *partition constant* (3.16), *partition ratio* or *distribution ratio* (3.5).

3.16 Partition Constant (K^o_D)

The ratio of activity of a given species A in the extract to its activity in the other phase with which it is in equilibrium, thus

$$(K^o_D)_A = a_{A,org}/a_{A,aq}$$

Its value should not vary with composition but depends on the choice of standard states and on the temperature (and eventually the pressure).

Note: See *transfer activity coefficient* (3.28).

3.17 Partition Ratio (K_D)

The ratio of the concentration of a substance in a single definite form, A, in the *extract* (4.8) to its concentration in the same form in the other phase at equilibrium, e.g. for an aqueous/organic system

$$(K_D)_A = [A]_{org}/[A]_{aq}$$

Notes:
(i) K_D is sometimes called the *distribution constant*; this is a good synonym. The terms *distribution coefficient*, *distribution ratio* (3.5), *partition constant* (3.16) and *extraction constant* (3.9) should not be used as synonyms for *partition ratio*.
(ii) The use of the inverse ratio (aqueous/organic) may be appropriate in certain cases, e.g. where the organic phase forms the *feed* (4.11) but its use in such cases should be clearly specified. The ratio of the concentration in the denser phase to the less dense phase is not recommended as it can be ambiguous.
(iii) If the pure *solvent* and infinitely dilute feed are taken as the standard state, $K_D \rightarrow K_D^\circ$ as the total concentration of dissolved materials decreases.

3.18 $pH_{0.5}$ or $pH_{1/2}$

That value of pH in an aqueous phase at which the *distribution ratio* (3.5) is unity at equilibrium.

Note: 50% of the solute is extracted ($E = 0.5$) *only* when the *phase ratio* (3.19) is unity.

3.19 Phase Ratio (in Liquid-liquid Distribution) (r)

The ratio of the quantity of the solvent (2.12) to that of the other phase.

Notes:
(i) Unless otherwise specified the phase ratio refers to the *phase volume ratio*.
(ii) If other aspects of the phase ratio are employed viz. *phase mass ratio*, *phase flow ratio*, these should be specified.

3.20 Recovery Factor

This term is not recommended. *Fraction extracted* (3.11) should be used.

3.21 Saturation Capacity See *Loading Capacity (3.12)*

3.22 Saturation Loading See *Loading Capacity (3.12)*

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3.23 Selectivity Coefficient

This term should not be used as a synonym for *separation factor* (3.26).

Note: This term has a specific meaning in relation to ion exchange by solid exchangers.

3.24 Selectivity Ratio

Synonym for *selectivity coefficient* (3.23). It should not be used as a synonym for *separation factor* (3.26).

3.25 Separation Coefficient

This term is not recommended. A synonym for *separation factor* (3.26).

3.26 Separation Factor (in Liquid-liquid Distribution) ($\alpha_{A,B}$)

The ratio of the respective *distribution ratios* (3.5) of two extractable solutes measured under the same conditions.

$$\alpha_{A,B} = D_A/D_B$$

Notes:
(i) By convention the solutes designated as A and B in the above are chosen so as to make $\alpha > 1$.
(ii) The term *separation coefficient* is not recommended.
(iii) The terms *selectivity coefficient* (3.23) and *selectivity ratio* (3.24) are not synonymous and should not be used.

3.27 Stoichiometric Capacity See *Ultimate Capacity (3.29)*

3.28 Transfer Activity Coefficient (γ_t)

A term used to quantify the difference in the free energy of a solute ion in two different standard states often in two different liquid phases. The relationship is $\Delta_t G^\circ = v\ RT \ln \gamma_t$ where $\Delta_t G^\circ$ is the transfer Gibbs energy and v is the number of ions in the solute. See *partition constant*.

Notes:
(i) See *IUPAC Information Bulletin* No. 34 (1974) [12] for full details.
(ii) It should not be confused with the *mass transfer coefficient* which represents the specific *rate* of transfer of a species from one phase to another.
(iii) It does not necessarily imply the physical transfer of a solute between two liquid phases.

3.29 Ultimate Capacity

The theoretical maximum capacity of a *solvent* (2.12) containing a given concentration of *extractant* (2.8) for a solute under any conditions.

Note: Where appropriate the term *stoichiometric capacity* can be used.

4. Process Terminology

4.1 Back Extraction

A synonym for *stripping* (by extraction) (4.43).

4.2 Back Washing

Often used as a synonym for *stripping* (4.43). This term is not recommended.

4.3 Continuity Inversion

A change in the mutual dispersion of two phases in contact. See *inversion* (4.13).

4.4 Crowding

The displacement of an impurity from an extract phase by contact with a solution containing the main extractable solute. See *scrubbing* (4.23), *exchange extraction* (4.8).

Note: The main solute need not be present in a pure solution but should have a higher *distribution ratio* (3.5) than the impurities present.

4.5 Crud

A deposit or emulsion at the interface between two partially settled phases.

Notes:
(i) The phenomenon of crud formation arises from many causes and this definition does not imply any single one.
(ii) Other terms – some unprintable – have been used but *crud* is the generally accepted term.

4.6 Density Inversion

The interchange of the denser and less dense phases due to changes in solute concentration. See *inversion* (4.13).

Note: *Phase inversion* (4.20) is often used in this context but is ambiguous.

4.7 Differential Contactor

A type of continuous multistage extraction equipment in which there is only one interface at which phase separation by settling occurs. See *theoretical stage* (4.52).

4.8 Exchange Extraction

An extraction operation or process in which a metal from one phase is exchanged with the equivalent amount of a second metal from the other phase. See *crowding* (4.4).

Note:
(i) This term may be used in connection with any step (e.g. *loading*, (4.16), *scrubbing* (4.23) or *stripping* (4.43) in a process).
(ii) This applies also to organic or molecular species.

4.9 Extraction (in Process Liquid-liquid Distribution)

In connection with processes, this term often refers to the initial transfer step whereby the *main solute* (1.13), often together with impurities, is transferred from *feed* to *solvent* (2.12). See *loading* (4.16).

Notes:
(i) *Partition and distribution* (1.4) are not synonyms in this specific instance.
(ii) The term *extraction* may be used in a more general sense. See under "General Definitions" (1.9).

4.10 Extraction Isotherm See *Distribution Isotherm (1.5)*

4.11 Feed

A solution introduced into an *extraction* system.

Note: It should be clearly identified (e.g. *scrub feed*) but, if used without qualification, it may be taken to designate the initial liquid phase containing the main solute to be transferred.

4.12 Height Equivalent to a Theoretical Stage (HETS)

See explanation of *Theoretical Stage* (4.52).

4.13 Inversion (or Phase Inversion)

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This term is used in two senses which should be specified.

(i) *density inversion* (4.6)
(ii) *continuity inversion* (4.3)

4.14 Load (in Liquid-liquid Distribution) (Verb)

To transfer solute from a *feed* (4.11) to another liquid phase.

4.15 Loaded Solvent See *Extract (2.7)*

Note: This term is usually used to denote the *extract* (2.7) after completion of a particular step, e.g. *extraction* or *scrubbing* (4.23)

4.16 Loading (Noun)

The concentration of an extracted solute in the *extract* (2.7).

4.17 Loading (Verb) *See Load (4.14)*

Note: Used in this sense the term normally refers to the operation of transferring the *main solute* (1.13)), often with impurities from the feed to the *solvent* (2.12).

4.18 O.K. Liquor

Sometimes used as a synonym for *strip product solution* (4.48) or *strip liquor* (4.42)

Note: This term is confusing and **should not** be used.

4.19 Operating Line

A graphical representation of the mass balance relationship of a solute across an extraction process *step* (4.41) or *stage* (4.38).

4.20 Phase Inversion **See *Density Inversion (4.6)***

4.21 Raffinate

The phase remaining after extraction of some specified solute(s). *When necessary* it should be further specified, e.g. *scrub raffinate* (4.30).

Note: The original meaning of *raffinate* as a "refined product" has become extended and changed by common usage.
The term should normally be applied only to waste streams but the latter may form the feed to a further extraction process for another solute.

4.22 Regeneration **See *Solvent Regeneration (4.37)***

4.23 Scrubbing **See *Crowding (4.2) and Selective Stripping (4.33)***

The process of selectively removing contaminating solutes (impurities) from an *extract* (2.7) that contains these as well as the *main extractable solute* (1.13) by treatment with a new immiscible liquid phase.

Note: The term *stripping* (4.43) has a different meaning and should not be used in this sense although this usage has been customary in certain industries.

4.24 Scrubbing Agent

The chemical reagent used to effect *scrubbing* (4.23).

Note: Often used as a synonym for its solution.

4.25 Scrubbing Agent Solution

The solution used to effect *scrubbing* (4.23)

Note: The term *scrub solution* is ambiguous and is not recommended.

4.26 Scrubbing Isotherm **See *Distribution Isotherm (1.5)***

4.27 Scrub Feed

The *extract* (2.7) to be scrubbed.

4.28 Scrub Liquor **See *Scrub Raffinate (4.30)***

Note: This term is ambiguous and is not recommended.

4.29 Scrub Product Solution

The solution that results from the *scrubbing* of impurities from an extract phase.

Note: The term *scrub liquor* is also used but can be confused with the *scrubbing agent solution* (4.25) and is not recommended. See *scrub raffinate* (4.30).

4.30 Scrub Raffinate

This term should only be used where the product solution from scrubbing is discharged to waste. *Scrub product solution* (4.29) is better where this stream is combined with *feed* (4.11) to the loading section.

4.31 Scrubbing Ratio **See *Distribution Ratio (3.5)***

Note: The term *scrubbing coefficient* is not recommended. This term is not common.

4.32 Scrub Solution **See *Scrubbing Agent Solution (4.25)***

Note: This term should not be used as it is ambiguous and can be confused with *scrub raffinate* (4.30) or *scrub product solution* (4.29).

4.33 Selective Scrubbing See *stripping (4.43)*

4.34 Solvent Inventory

The total quantity of solvent present in the process.

4.35 Solvent Loss

The total quantity of solvent lost during the operation of a process.

Note: There are a number of ways currently in use to express both *solvent inventory* and *solvent loss* and authors should carefully define how they are using the terms until a generally agreed procedure can be recommended.

4.36 Solvent Purification

See *solvent regeneration*. The description *solvent purification* naturally applies also to the purification of fresh *solvent* (2.12).

4.37 Solvent Regeneration

Treatment of the solvent for re-cycling, e.g. by removal of degradation products or non-strippable solutes.

Note: The term *solvent purification* is synonymous, but the terms *scrubbing* (4.23), *stripping* (4.31) and *washing* should not be used in this context.

4.38 Stage

That physically distinct part of an extraction process in which transfer of solute(s) occurs, followed by phase separation. See *theoretical stage* (4.52).

Notes:
(i) For certain types of equipment with a single phase separation interface, the term *theoretical stage* (4.52) is more appropriate.
(ii) Equilibrium need not necessarily be established in a stage.

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4.39 Stagewise Contactor

A type of continuous multi-stage liquid–liquid contactor in which each stage has a physically distinct cycle of interphase contact and separation.

Note: There will be the same number of phase separation interfaces as there are stages.

4.40 Steady State (in Liquid-liquid Distribution)

The state of a continuous process when it is operating in such a way that the concentration of solutes in exit streams remains constants with respect to time for constant feed concentrations, even though the two phases are not necessarily in thermodynamic equilibrium in any part of the process.

Note: The term *equilibrium* should not be used to describe this situation.

4.41 Step (in Liquid-liquid Distribution)

That operation in an overall extraction process in which transfer of solute(s) occurs in a particular direction, e.g. *Loading* (4.16), *stripping* (4.43), *scrubbing* (4.23).

4.42 Strip Liquor

A liquid phase resulting from the operation of *stripping* (4.43). See *strip solution* (4.50) and *strip raffinate* (4.49).

Notes:
(i) This term is ambiguous and should be used carefully. *Strip raffinate* (4.49) is more appropriate.
(ii) The term *O.K. Liquor* (4.18) is not recommended.

4.43 Stripping

The process of removing solute(s) from a *loaded solvent* or *extract* (2.7). Generally this refers to the main solute(s) present.

Notes:
(i) Where appropriate, e.g. when liquid-liquid distribution is used for *stripping*, the term *back-extraction* can be used. The terms *back-washing* and *re-extraction* (1.17) are not recommended.
(ii) The recent application of *selective stripping* of solutes as a separation method leads to some confusion between the terms *stripping* and *scrubbing* (4.23). It is recommended that the term *scrubbing* be reserved for the operation of removing contaminants (impurities) from an *extract* (2.7) (where the *scrub raffinate* (4.30) is often recycled to the loading step) and the term *selective stripping* be used where two or more main solutes are stripped successively from an *extract*, usually with different *stripping agents* (4.44), with a view to their subsequent separate recovery from solution for analysis.

4.44 Stripping Agent

The active substance effective in *stripping* (4.43).

4.45 Stripping Agent Solution

The liquid phase used to accomplish *stripping* (4.43).

4.46 Stripping Ratio See *Distribution Ratio (3.5)*

Notes:
(i) This term is usually defined as the inverse ratio to the *distribution ratio* (3.5, comment iii), i.e. in aqueous-organic systems the aqueous phase concentration of solute is the numerator and the organic phase concentration the denominator. Their usage should be clearly defined.
(ii) The term *stripping coefficient* is not recommended.

4.47 Stripping Ratio See *Distribution Isotherm (1.5), Equilibrium Line (1.7)*

Note: In the graphical representation of *stripping isotherms*, the axes are often interchanged from those used to represent the phases for *extraction isotherms*. It is essential that the axes be clearly labelled.

4.48 Strip Product Solution

The liquid phase resulting from *stripping* (4.43) of a *solvent* (2.12). See *stripping liquor* (4.42), *strip solution* (4.50), *strip raffinate* (4.30), *O.K. liquor* (4.18).

Note: The last four terms are not recommended.

4.49 Strip Raffinate

This term is not recommended. *Raffinate* (4.21) should be reserved for waste streams and the liquid phase resulting from stripping normally contains the desired product.

4.50 Strip Solution

The liquid phase used for *stripping* (4.43).

Note: There is some ambiguity between the terms *strip liquor* and *strip solution*. Perhaps *strip product solution* (4.48) would be more appropriate to the former and *stripping agent solution* (4.45) for the latter. See *stripping agent* (4.44).

4.51 Tenor

A term sometimes used to denote the concentration levels of various solutes in the *feed* (4.11). It is not recommended.

4.52 Theoretical Stage

That part of a continuous multi-stage contactor in which the amount of solute transferred from one phase to the other is equivalent to that which would be transferred in an actual stage at equilibrium under comparable conditions of solute concentration in each phase as determined from the *distribution isotherm* (1.5) and *operating line* (4.19) for the system.

Note: Thus from the number of theoretical stages so determined and the height of the contactor the *height equivalent to a theoretical stage* (HETS) may be calculated.

4.53 Washing See solvent regeneration (4.37)

Note: This term is vague and is not recommended.

Table 1 Index of terms

Accelerator	2.1	Partition coefficient	3.15
Antagonism	1.1	Partition constant	3.16
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Conditioning	1.3	Regeneration	4.22
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Cosolvent	2.4	Re-extraction	1.17
Crowding	4.4	Salting out	1.18
Crud	4.5	Saturation capacity	3.21
Decontamination factor	3.2	Saturation loading	3.22
Density inversion	4.6	Scrubbing	4.23
Differential contactor	4.7	Scrubbing agent	4.24
Diluent	2.5	Scrubbing agent solution	4.25
Distribution	1.4	Scrubbing isotherm	4.26
Distribution coefficient	3.3	Scrub feed	4.27
Distribution constant	3.4	Scrub liquor	4.28
Distribution isotherm	1.5	Scrub product solution	4.29
Distribution ratio (in liquid-liquid distribution)	3.5	Scrub raffinate	4.30
Enrichment factor (in liquid-liquid distribution)	3.6	Scrubbing ratio	4.31
Epi-phase	2.6	Scrub solution	4.32
Equilibration	1.6	Selectivity coefficient	3.23
Equilibrium line	1.7	Selectivity ratio	3.24
Exchange extraction	4.8	Selective stripping	4.33
Extract (noun)	2.7	Separation coefficient	3.25
Extract (verb)	1.8	Separation factor (in liquid-liquid distribution)	3.26
Extractability	3.7	Solvent	2.12
Extractant	2.8	Solvent extraction	1.19
Extraction	1.9	Solvent inventory	4.34
Extraction (in process liquid-liquid distribution)	4.9	Solvent ion exchange (six)	1.20
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Liquid ion exchange	1.10	Stripping	4.43
Liquid-liquid distribution (extraction) (partition)	1.11	Stripping agent	4.44
Load (in liquid-liquid distribution) (verb)	4.14	Stripping agent solution	4.45
Loaded solvent	4.15	Stripping ratio	4.46
Loading (noun)	4.16	Stripping isotherm	4.47
Loading (verb)	4.17	Strip product solution	4.48
Loading capacity	3.12	Strip raffinate	4.49
Macro-element	1.12	Strip solution	4.50
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Mass distribution ratio	3.13	Substoichiometric extraction	1.22
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Modifier	2.11	Theoretical stage	4.52
O.K. Liquor	4.18	Transfer activity coefficient	3.28
Operating line	4.19	Ultimate capacity	3.29
Partition	1.15	Washing	4.53

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Table 2 Index of symbols

D	Distribution ratio (in liquid-liquid distribution)	3.5
S	Enrichment factor (in liquid-liquid distribution)	3.6
D_m	Extraction factor	3.10
K^o_{ex}	Extraction (equilibrium) constant at zero ionic strength	3.9
E	Fraction extracted	3.11
K^o_d	Partition constant	3.16
K_d	Partition ratio	3.17
r	Phase ratio (in liquid-liquid distribution)	3.19
$\alpha_{A,B}$	Separation factor (in liquid-liquid distribution)	3.26
γ_t	Transfer activity coefficient	3.28

Appendix 1. Comparison of Nomenclature With Previously Defined Terms

(OB, Orange Book [9]; Chrom, Nomenclature for Chromatography [10]

Carrier (2.12) This term is not recommended in this area (OB p54)
Catalyst (*in liquid-liquid distribution*) (2.3) Defined as a specific use of *catalyst* (OB p56).
Diluent (2.5) Redefined from OB 9.2.4 and 9.2.10 in a more general sense
Distribution (1.4) Now defined – only mentioned in OB 9.2.6
Distribution coefficient (3.3) Not recommended in this area (OB 9.4.10)
Distribution constant (3.4) Matches uses in Chrom 3.9 and 5.6.
Distribution ratio (*in liquid-liquid distribution*) (3.5) Slight clarification of usage from OB 9.2.6
Enrichment factor (*in liquid-liquid distribution*) (3.6) Rewording of OB 9.2.8 to make more general.
Extractant (2.8) Redefined compared to OB 9.2.11
Extraction (*in liquid-liquid distribution*) (1.9) See more precise term OB 9.2.4
Extraction coefficient (3.8) Not recommended (OB 9.2.6)
Extraction constant (3.9) Slightly amended from OB 9.2.5
Liquid-liquid distribution (1.11) Redefined from OB 9.2.4
Mass distribution ratio (3.13) Unchanged from OB 9.4.10. Not recommended in Chrom 3.7.12.
Modifier (2.11) Term now defined (see OB 9.2.4)
Partition (1.15) Term now defined (OB 9.2.1)
Partition coefficient (3.15) and *partition constant* (3.16) Not recommended (OB 9.2.6) agrees 3.9.01
Recovery factor (3.20) Now not recommended (OB 9.2.7)
Salting out (1.18) Definition broadened from OB 9.2.15
Selectivity coefficient (3.23) Not recommended in this area (used in Chrom 5.5.02)
Separation factor (*in liquid-liquid distribution*) (3.25) Specifically defined for this area to distinguish from Chrom 3.7.14.2 and 5.5.04
Solvent (*in liquid-liquid distribution*) (2.12) Specific definition provided for this area more limited than OB 9.1.2 and redefines 9.2.9. Differs from Chrom 1.1.11 and 5.2.01

Appendix 2. Survey of Partition Terminology Used by Authors of Books

Term: Activities of a single species $\frac{a_{A,org}}{a_{A,aq}}$

Symbol	Name	Reference
K_D°	Partition constant	9
P°	Activity partition constant	13
P	Partition coefficient or Distribution coefficient	14, 15
K_p	Thermodynamic partition constant	16
p° or K_p°	Thermodynamic partition constant	17
P	Thermodynamic partition coefficient or Partition coefficient	18
K_D	Distribution coefficient	19
K	Distribution coefficient	15

Term: Total concentration of related species $\frac{(C_A)_{org}}{(C_A)_{aq}}$

Symbol	Name	Reference
D_c	Concentration distribution ratio	9, 16, 31
D	Distribution ratio	14, 19, 20, 22, 23, 25, 26, 27, 31, 33, 34, 37
D	Distribution coefficient	17, 18, 37, 38
D^{Total}	Distribution coefficient	34
q	Distribution coefficient	11
Q	Extraction coefficient	39
E	Extraction coefficient	36
E	Distribution ratio	17, 35

Term: Concentration distribution of $\frac{[A]_{org}}{[A]_{aq}}$ a single species

Symbol	Name	Reference
K_D	Distribution constant	9, 20, 21
K_D	Distribution coefficient	21, 22, 23, 24
K_D	Distribution or partition coefficient	25
K_D	Partition coefficient	26
K_D	Partition constant	27
K	Partition coefficient	14, 28, 29
K or λ	Partition ratio	30
K	Partition or Distribution coefficient	31
K	Distribution coefficient	15
K_p	Partition coefficient	16
P	Partition constant or coefficient	32
P	Partition coefficient or distribution constant	33
P	Partition ratio	17,18
D	Distribution ratio	11,34
Q	Partition ratio	35
Q_c	Molar partition constant	36

Term: Equilibrium constant for:

$$M_{aq}^{n+} + nHL_{org} \rightleftharpoons ML_{n,org} + nH_{aq}^{+}$$

$$\text{i.e.} = \frac{[ML_n]_{org} \times [H^+]_{aq}^n}{[M^n]_{aq}^+ \times [HL]_{org}^n}$$

Symbol	Name	Reference
K_{ex}°	Extraction constant at zero ionic strength (activities in above)	9
K_{ex}	Extraction constant or Overall extraction constant	9, 19, 20
K_{ext}	Extraction equilibrium constant	32
K	Extraction constant	39
K'_{ex}	Conditional extraction constant	11

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12C. Non-Linear Chromatography (IUPAC Recommendations 1996)

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